



Log P (Partition Coefficient) & Use in Strata-X Reverse Phase SPE method Development

Definition of Log P (Partition Coefficient)

A partition coefficient is the ratio of concentrations of an un-ionized compound in the two phases of a mixture of two immiscible solvents at equilibrium.

Generally, the two solvents chosen are water (aqueous phase) and octanol (hydrophobic organic phase). To take this measurement, the compound to be measured is added to the water/octanol system. Once equilibrium has been achieved, the compound is quantified in each solvent via UV/VIS and the log P is expressed with this equation:

$$\log P_{oct/wat} = \log \left(\frac{[solute]_{octanol}}{[solute]_{water}^{un-ionized}} \right)$$

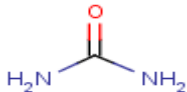
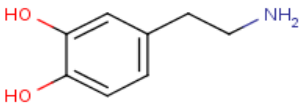
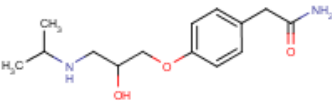
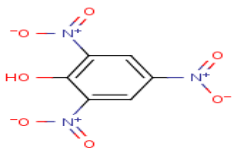
This value reflects how hydrophilic or hydrophobic an analyte is.

Log P = 1 means 10:1 Organic:Aqueous (Slightly Hydrophobic)

Log P = 0 means 1:1 Organic:Aqueous (Equally Hydrophobic/Hydrophilic)

Log P = -1 means 1:10 Organic:Aqueous (Slightly Hydrophilic)

To add further clarity on what a log P value of X means, here is a list of a range of compounds and their corresponding log P values. (Compounds are listed in increasing hydrophobicity):

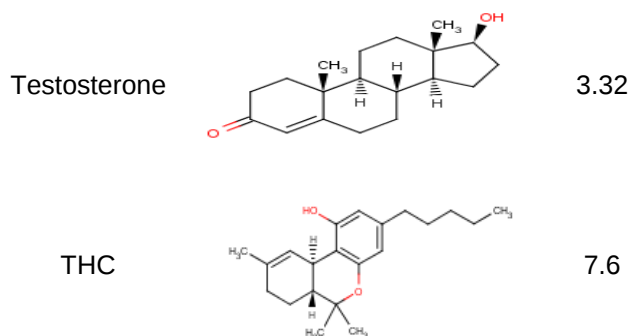
Compound	Structure	log P
Urea		-2.11
Dopamine		-0.98
Atenolol		0.16
Picric Acid		1.33

Key words: log P, Strata X, SPE

Author: Michael Rummel



Technical Tip



It is apparent in the structural make-up that urea is much more polar than testosterone, but the log P measurement helps quantify this (Testosterone is ~ 100,000 times more non-polar than urea).

Now let's look on how we can apply this knowledge to SPE method development.

Log P with Strata-X SPE Method Development - Reverse Phase

A successful SPE method operates via an on/off mechanism. i.e. will the compound of interest stick or not stick the media? The log P of a compound can be a useful tool to predict an answer to this question, specifically when developing a reverse phase SPE procedure.

- When using Strata-X, it is a general rule of thumb that it can retain un-ionized compounds with a log P > -1.0.
- Comparatively, Strata-C18-E can retain un-ionized compounds with a log P > +1.0.

Therefore, Strata-X is chosen when extracting moderately polar compounds. The n-vinyl pyrillidone modification on Strata-X allows for more polar selectivity and aids in the retention of these moderately polar compounds.

Let's now look at a specific example, urea. Out of the compounds listed above, the log P (-2.11) can be used to determine that neither Strata-X nor Strata-C18-E would work. Similarly, we can predict that Strata-C18-E would not be a good choice dopamine or atenolol, since both compounds log P's are < +1.0

The log P value can also be used to give an idea of wash strengths to recommend in a reverse phase SPE method. The higher the log P value, the better it will be retained allowing for a more aggressive wash. For example, testosterone can be washed up to 60% MeOH on Strata-X. Not too surprising as testosterone is a pretty hydrophobic molecule at a log P of 3.32. (For more information on testosterone SPE method development, see TN-0017)

In summation, the log P value serves as a useful guideline for SPE MD. Remember it is just a guideline and it should be used in conjunction with other analyte properties to determine a great starting SPE method.